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Progress Towards the Development of Transient Ram Accelerator Simulation as Part of the USAF Armament Directorate Research Program

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PREFACE

This work was funded by WL/MNSH of the Armament Directorate at Eglin AFB FL under the Ram Accelerator Research program. Capt Randall P. Drabczuk, WL/MNSH, and personnel from Science Applications International Corporation (SAIC) in Shalimar FL and Ft. Washington PA performed the work during the period of January 1992 to June 1992.

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PROGRESS TOWARDS THE DEVELOPMENT OF TRANSIENT RAM ACCELERATOR SIMULATION AS PART OF THE U.S. AIR FORCE ARMAMENT DIRECTORATE RESEARCH PROGRAM†

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ABSTRACT

This paper describes the development of an advanced computational fluid dynamic (CFD) simulation capability in support of the U.S. Air Force Armament Directorate's ram accelerator research initiative. The state-of-the-art CRAFT computer code has been specialized for high fidelity, transient ram accelerator simulations via inclusion of generalized dynamic gridding, solution adaptive grid clustering, high pressure thermochemistry, etc. Selected ram accelerator simulations are presented which serve to exhibit the CRAFT code's capabilities and identify some of the principal research/design issues.

INTRODUCTION

At an earlier AIAA meeting,[1] a new propulsive-oriented Navier-Stokes (NS) code, CRAFT, was introduced which was an extension of the TUFF aerodynamic NS code of Molvik and Merkle.[2] Applications of CRAFT to various combusting, multiphase flow problems were exhibited. In this paper, the simulation of ram accelerator flowfields with CRAFT will be discussed – a role undertaken in support of new research initiatives at the Armament Directorate of Wright Labs, U.S. Air Force.

The Armament Directorate of Wright Laboratories (WL/MN), located at Eglin Air Force Base, in conjunction with the Air Force Office of Scientific Research (AFOSR), has initiated a multi-year research program to advance the understanding of the basic physics of the ram accelerator. The research effort has three principal areas of focus:

(1) design and construction of a large-bore ram accelerator test facility at Eglin AFB;

(2) investigation of diagnostic techniques; and,

(3) development and execution of computational fluid dynamic (CFD) models.

The design of the ram accelerator research facility to be constructed at Eglin AFB has been initiated. Present plans call for the system to include a conventional powder gun injector, an evacuated vent chamber, an eighteen meter long ram accelerator section with a 90 mm bore diameter, and a catch-tank.

The diagnostic research will focus on schlieren, x-ray shadowgraph, emission spectroscopy, and a single-pulse imaging (Rayleigh scattering). The schlieren technique depends on the change in illumination due to the changes in refractive index (density gradients), which are made visible by introducing subsidiary elements into the optical system, such as a knife edge, resulting in the appearance of the intensity variations in the location of the focussed image. The x-ray technique depends on the change in the illumination due to absorption along the line of sight by the gas constituents, in a manner similar to optical shadowgraphy,[3-7] which examines the intensity variations in a plane which is not the plane of the focussed image. The interest in using x-rays derives from a need to have a method that operates successfully at high pressures. X-ray shadowgraphy has been utilized to observe density gradients in the flow as the pressure increases up to values in the kilobar regime. Emission spectroscopy will be employed to infer flowfield temperature and pressure, as well as composition. An anticipated difficulty with emission spectra is that the opacity of the flow system may increase rapidly with increasing pressure. The research will identify the pressure regime over which this technique will be useful. The final diagnostic technique to be investigated is single-pulse planar imaging. The primary focus will be on Rayleigh scattering, but potentially both Raman and Thompson scattering will be utilized.

High fidelity CFD simulations will be an integral part of the overall ram accelerator research program. CFD simulations will

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be used for conducting trade-off studies to support the in-house test facility design and development. A second objective of the computational fluid dynamics task is to support the development of the diagnostic techniques and data interpretation. The final and crucial longer term objective is to develop a detailed understanding of the complex physical and thermochemical processes governing the ram accelerator concept. This paper will provide a background of the CFD technique being utilized to support this research initiative and present preliminary findings.

Earlier simulations of ram accelerator flowfields have primarily emphasized a "snapshot" prediction of the ram flowfield, e.g., a steady-state simulation at a fixed trajectory point. Such studies include the work of Nusca at BRL,[8] Yungster and Eberhardt at the University of Washington,[9,10] Yungster at NASA Lewis,[11,12] Imlay et al. at AMTEC,[13] Humphrey and Sobota at APRI,[14] and Li, Kailasanath and Oran at NRL.[15] The work of Nusca, Yungster et al., and Imlay et al. has involved the use of modern finite-volume upwind/implicit numerics (e.g., higher-order Roe/TVD). Nusca has used uncoupled, global chemistry in an overlaid manner. Yungster and Imlay et al. have used loosely-coupled (diagonalized) finite-rate chemistry. Li et al. have utilized explicit FCT numerics with time-split global chemistry. With regard to turbulence modeling, Nusca, Yungster and Imlay et al. have employed algebraic models (e.g., Baldwin-Lomax), while Li et al. have not utilized a turbulence model (their work is Euler or viscous with "boosted" laminar viscosity).

A workshop was recently held at AFOSR with a primary purpose of identifying principal research issues and requirements for high fidelity CFD simulation of ram accelerator flowfields. The workshop group felt that a full transient simulation was requisite for studying the basic physics and thermochemistry of ram accelerators. Very little research has been done in this area. The only work to date using state-of-the-art upwind/implicit numerics to analyze transient hypervelocity interior ballistic flows is that of Sinha, Dash et al. as applied to Electro-Thermo-Chemical (ETC) guns.[16] Alternate transient interior ballistic flow simulation work for ram accelerators, for ETC guns, and for liquid propellant guns, has primarily involved the use of structured and unstructured explicit methods (which cannot efficiently treat thin boundary layers). The principal research areas identified at the workshop included numerics (e.g., dynamic adaptive gridding and advanced implicit/upwind algorithms), turbulence modeling in a transient environment (e.g., LES simulation), 3D effects (e.g., vortex shedding from fins) and combustion phenomenology in the high Re, high pressure ram accelerator environment.

The methodology in CRAFT is quite new and reflects "state-of-the-art" capabilities in this country. Principal milestones in the evolution of CRAFT are summarized in Table I. Our work with earlier NS codes such as PARCH[17,18] has indicated the requirement to develop specialized versions for specific applications.[19,20] This philosophy has been adhered to in our work with CRAFT. Specialized research versions of CRAFT developed to date are described in Table II. This paper will review the basic methodology available in CRAFT (equations and numerics) supplementing descriptions provided in earlier publications.[1,2] The problem specific features of the RAM version will be emphasized.

GAS-PHASE EQUATIONS

The Reynolds-Averaged Navier-Stokes equations integrated by the RAM version of CRAFT are listed in Table III. They include chemical species equations for the species mass fractions ρ_i, and turbulence model equations for the turbulent kinetic energy, k, and turbulence dissipation rate parameter, ϵ. The source terms in D provide for chemical non-equilibrium ($\dot{\omega}_i$), and turbulence non-equilibrium ($\mathcal{P}$-$\rho\epsilon$) where $\mathcal{P}$ is the production term for turbulent kinetic energy. The viscous fluxes include full cross-flow stress terms which is requisite for solving 3D problems, e.g., projectile with fins. A two-equation kϵ turbulence model[21] has been incorporated in a strongly coupled, implicit manner. Near-wall effects have been dealt with via the low Reynolds number formulation of Chien[22] and the recent model of Rodi.[23] High-speed compressibility issues have been accounted for via the upgrades of Dash et al.[24] based on "compressible dissipation" concepts introduced by Sarkar[25] and Zeman.[26] The CRAFT code contains generalized, multi-component/multi-step, finite-rate chemical kinetics. The species production/destruction rates are determined via the law of mass action and chemical reaction rate constants are expressed in Arrhenius form. The code accesses a JANNAF-based thermochemical/transport databank whose features mimic those in standardized codes such as SPF.[27] The databank contains thermodynamic and transport data curve fits for varied species and rate constants for pertinent chemical reactions.

NUMERICAL PROCEDURES

The CRAFT code is an extended propulsive-oriented derivative of the TUFF aerodynamic code which was formulated as a thin-layer NS code within a finite-volume framework, with higher-order upwind inviscid fluxes based on the approximate Riemann solver of Roe.[28] The numerics incorporate TVD procedures outlined by Chakravarthy[29] to eliminate spurious oscillations generally associated with higher order upwind schemes. The fluid and species equations are strongly coupled, and the solution is made fully implicit by linearizing all convective/diffusive fluxes as well as the chemical source term (with respect to all dependent variables, not just chemical species as in other codes of this type). An ADI splitting is employed. A modified Newton iteration is employed to eliminate linearization errors in the iterative process. Elimination of linearization/factorization errors was recently shown by Ridder and Beddini[30] to be essential for accurately representing complex wave propagation phenomena in a non-diffusive manner, as requisite for acoustic applications and instability phenomena.

The incorporation of nonequilibrium kinetics has followed the finite-volume, fully-implicit philosophy of the gas dynamics. In departure from earlier generation explicit and loosely coupled schemes, the species and fluid dynamic equations are strongly coupled and simultaneously solved, readily allowing information transfer between the two sets of equations. In contrast, the

Table I. Evolution of Methodology in CRAFT Code

- UPWIND/IMPLICIT FINITE-VOLUME METHODOLOGY (ROE/TVD) APPLIED TO EXTERNAL AERODYNAMIC FLOWFIELDS ~ 1986-1988. Reference: Walters and Thomas, "Advances in Upwind Relaxation Methods," *State of the Art Surveys on Computational Fluid Mechanics*, ASME Pub., 1988.
- EXTENSIONS OF ROE/TVD METHODOLOGY TO MULTI-COMPONENT/REAL GAS FLOWS WITH CHEMICAL/THERMAL NONEQUILIBRIUM ~ 1988-1989. Reference: Liu and Vinokur, "Upwind Algorithms for General Thermo-Chemical Nonequilibrium Flows," *AIAA Paper 89-0201, Jan. 1989.*
- EXPLORATORY STUDIES OF ROE/TVD NUMERICS FOR UNSTEADY FLOWS, ACCURATE WAVE PROPAGATION IN DUCT (RESONANCE TUBE) ~ 1989. Reference: Ridder and Beddini, "Time-Accurate Finite-Volume Method for Propulsion Chamber Flows," AIAA Paper 89-2554, July 1989.
- EXTENSIONS OF ROE/TVD METHODOLOGY FOR PROPULSIVE FLOWS WITH COMBUSTION CHEMISTRY, ADVANCED TURBULENCE MODELS ~ 1989-1991. Reference: Dash, "Advanced Computational Models for Analyzing High-Speed Propulsive Flowfields," *1990 JANNAF Propulsion Meeting*, Oct. 1990.
- EXTENSIONS OF ROE/TVD METHODOLOGY FOR UNSTEADY ROCKET PLUME PROBLEMS WITH GAS/PARTICLE NONEQUILIBRIUM ~ 1989-1991. Reference: Sinha, Hosangadi and Dash, "The CRAFT NS Code and Preliminary Applications to Unsteady, Reacting, Multi-Phase Plume Flowfield Problems," *1991 JANNAF Plume Meeting*, May 1991.
- EXPLORATORY STUDIES OF ROE/TVD METHODOLOGY FOR GUN FLOWFIELDS WITH DYNAMIC GRID EXTENSIONS ~ 1990-1991. Reference: Hosangadi and Sinha, "Development of a Dynamic Grid Navier-Stokes Solver for Computing Electro-Thermo-Chemical Gun Configurations," SAIC/TR-88, Dec. 1990.
- EXTENSIONS OF ROE/TVD METHODOLOGY FOR GAS/LIQUID MIXTURES FOR ETC GUN FLOWFIELD SIMULATION ~ 1992. Reference: Sinha, Hosangadi, York and Dash, "First Principles Two-Dimensional Modeling of ETC Interior Ballistics," *29th JANNAF Combustion Meeting*, October 1992.

Table II. Research Versions of CRAFT NS Code

CODE NAME	CRAFT/JR	CRAFT/ETC	CRAFT/RNP	CRAFT/LU	CRAFT/RAM
APPLICATION	High-Speed Jet Research	ETC Gun Flowfields	Rocket Nozzles/ Plumes	Numerical Research	Ram Accelerator Flowfields
SPONSOR	NASA/LaRC, HSRP	BRL	MICOM	Internal Research	AFOSR & WL/MNSH
EQUATIONS	1D/2D/AXI/3D	1D/2D/AXI/3D	1D/2D/AXI/3D	1D/2D/AXI/3D	1D/2D/AXI/3D
CHEMISTRY	Perfect Gas, Two-Stream	Imperfect Gas, Combustion Chemistry, Multi-Phase Chemistry	SPF Finite-Rate Chemistry, Two-Stream, Perfect Gas	Perfect Gas	Imperfect Gas, Finite-Rate Detailed Kinetics
TURBULENCE	k-ε, Compressibility Extensions, ARS Extensions	k-ε	k-ε/Chien, Compressibility Extensions	k-ε	k-ε/Chien, Advanced Compressibility Corrections
PARTICULATES	None	Equilibrated Mixture, Nonequilibrium Liquid Propellants	Nonequilibrium	None	None
SOLUTION	Implicit/Upwind (Roe/TVD) Strongly-Coupled Fluid/Species/ Turbulence (8 x 8 Block Inversion), Time-Accurate or Time-Asymptotic	Implicit/Upwind (Roe/TVD) on Dynamic Grid, Time-Accurate Solution, Strongly-Coupled Equations, Variable Matrix Size	Implicit/Upwind (Roe/TVD) on Fixed Grid, Time-Accurate or Time-Asymptotic, Strongly-Coupled Equations, Variable Matrix Size	LU Upgrade for Robustness, Faster Convergence (CFL ~ 25-50)	Implicit/Upwind (Roe/TVD) on Dynamic Grid, Time-Accurate Solution, Strongly-Coupled Equations, Variable Matrix Size
NEW WORK	Exploring New Turbulence Models, New Non-Reflective BC	Inclusion of Liquid Phase, Gas/Liquid Interface, Droplet Formation Model	Adaptive Gridding for Unsteady Multi-Phase Flows	Rewrite of Code Structure to Optimize LU Storage for 3D	Adaptive, Dynamic Gridding for Unsteady Flows, LES

Table III. CRAFT NS Equations

$$\frac{\partial}{\partial t}\iiint Q\,dV + \iint (E_{i+1/2} - E_{i-1/2})\,d\eta\,d\zeta$$

$$+ \iint (F_{j+1/2} - F_{j-1/2})\,d\xi\,d\zeta + \iint (G_{k+1/2} - G_{k-1/2})\,d\xi\,d\eta$$

$$= \frac{1}{Re}\iint (R_{i+1/2} - R_{i-1/2})\,d\eta\,d\zeta + \iint (S_{j+1/2} - S_{j-1/2})\,d\xi\,d\zeta$$

$$+ \frac{1}{Re}\iint (T_{k+1/2} - T_{k-1/2})\,d\xi\,d\eta + \iiint D\,dV$$

$$Q = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \\ \rho_1 \\ \rho_2 \\ \rho_{n-1} \\ \rho k \\ \rho \epsilon \end{pmatrix} ; E = \begin{pmatrix} \rho\hat{U} \\ \rho\hat{U}u + \xi_x P \\ \rho\hat{U}v + \xi_y P \\ \rho\hat{U}w + \xi_z P \\ (e+P)\hat{U} \\ \rho_1\hat{U} \\ \rho_2\hat{U} \\ \rho_{n-1}\hat{U} \\ \rho\hat{U}k \\ \rho\hat{U}\epsilon \end{pmatrix} ; D = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_1 \\ \dot{\omega}_2 \\ \vdots \\ \dot{\omega}_{n-1} \\ P - \rho\epsilon \\ \frac{\epsilon}{k}(C_1 P - C_2 \rho\epsilon) \end{pmatrix} ; R = \begin{pmatrix} 0 \\ \xi_x\tau_{xx} + m_y\tau_{xy} + n_z\tau_{xz} \\ \xi_x\tau_{yx} + m_y\tau_{yy} + n_z\tau_{yz} \\ \xi_x\tau_{yz} + m_y\tau_{zy} + n_z\tau_{zz} \\ \xi_x\beta_x + m_y\beta_y + n_z\beta_z \\ \mu(\xi_x\rho_{1x} + m_y\rho_{1y} + n_z\rho_{1z}) \\ \vdots \\ \mu(\xi_x\rho_{nx} + m_y\rho_{ny} + n_z\rho_{nz}) \\ \mu(\xi_x k_x + m_y k_y + n_z k_z) \\ \mu(\xi_x \epsilon_x + m_y \epsilon_y + n_z k_z) \end{pmatrix}$$

$$\begin{aligned}
\tau_{xx} &= \lambda(u_x + v_y + w_z) + 2\mu u_x \\
\tau_{xy} &= \tau_{yx} = \mu(u_y + v_x) \\
\tau_{xz} &= \tau_{zx} = \mu(u_z + w_x) \\
\beta_x &= -KT_x + u\tau_{xx} + v\tau_{xy} + w\tau_{yz} \\
\beta_y &= -KT_y + u\tau_{yx} + v\tau_{yy} + w\tau_{yz} \\
\beta_z &= -KT_z + u\tau_{yz} + v\tau_{zy} + w\tau_{zz} \\
\lambda &= -\tfrac{2}{3}\mu
\end{aligned}$$

IN THE ABOVE EQUATIONS, $\xi(x,y,z)$, $\eta(x,y,z)$, $\zeta(x,y,z)$, REPRESENT THE CURVILINEAR COORDINATES IN THE TRANSFORMED COMPUTATIONAL SPACE, THE METRICS ℓ_x, ℓ_y, ℓ_z ARE THE COMPONENTS OF THE CELL FACE NORMAL $\vec{\ell}$, POINTING IN THE POSITIVE ξ DIRECTION WITH LENGTH EQUAL TO CELL FACE AREA. SIMILARLY THE OTHER METRIC QUANTITIES ARE THE COMPONENTS OF THE VECTORS m AND n, WHICH ARE THE NORMAL VECTORS OF THE CORRESPONDING m, AND n. THE FLUID PROPERTIES ARE GIVEN BY THE DENSITY ρ, CARTESIAN VELOCITY COMPONENTS (u, v, w), AND THE TOTAL ENERGY PER UNIT VOLUME, e, AND SPECIES CONCENTRATIONS, ρ_i. THE TRANSPORT PROPERTIES ARE GIVEN BY μ BEING THE LAMINAR VISCOSITY, γ BEING THE RATIO OF SPECIFIC HEATS, AND K BEING THE THERMAL CONDUCTIVITY. THE TURBULENCE EQUATIONS ARE DERIVED IN TERMS OF THE TURBULENT KINETIC ENERGY, k, AND THE DISSIPATION RATE, ϵ. THE CONTRAVARIANT VELOCITY COMPONENTS ARE DEFINED AS FOLLOWS:

$$\begin{aligned}
\hat{U} &= \ell_x u + \ell_y v + \ell_z w \\
\hat{V} &= m_x u + m_y v + m_z w \\
\hat{W} &= n_x u + n_y v + n_z w
\end{aligned}$$

FOR TURBULENT FLOW SIMULATION, THE LAMINAR VISCOSITY AND THE THERMAL CONDUCTIVITY ARE REPLACED BY THE RESPECTIVE SUMS OF LAMINAR AND TURBULENT VALUES. THE k-ϵ TURBULENCE MODEL CONSTANTS WHICH HAVE BEEN USED ARE $C_\mu = .09$, $C_1 = 1.44$ and $C_2 = 1.92$.

earlier techniques separately solved the two sets of equations which reduces the computational effort but severely inhibits the flow of information. This can be a severe handicap for strongly combusting flows, e.g., blast waves, gun chamber flowfields, etc., where significant coupling exists between the chemical release of energy and flowfield pressurization. A major breakthrough has been the pioneering work of Vinokur and Liu[31] in reformulating the original "perfect gas" Roe scheme and the associated Reimann problem to account for multi-component, real gas flow with chemical and thermal nonequilibrium.

The extension of CRAFT to include a two-equation ke turbulence model is a straightforward extension of the basic finite-volume based upwind/TVD methodology. The turbulence model equations are cast as a part of the strongly-coupled equation set for enhanced accuracy and robustness. The implicit treatment is extended to the turbulence nonequilibrium source terms to eliminate "stiffness." This is requisite for handling the low Reynolds number near wall terms. The linearization of source terms is a somewhat inexact procedure and several strategies have been developed. Instead of a brute force mathematical treatment, the linearization is being guided by turbulence behavior typical of low Reynolds number near wall regions and high Reynolds number free shear zones. Various methods are being explored to identify the optimal technique for propulsive/plume flowfields. In addition, the selection of appropriate background levels for freestream fluctuation intensity and length scale have been found to be sensitive parameters and must be judiciously specified.

DYNAMIC GRID UPGRADES

As a preliminary step towards developing a gun capability, CRAFT was upgraded to allow for unsteady simulations with a moving projectile and thus an ever expanding and/or moving gun chamber computational domain. The generalized dynamic grid formulation incorporated enhances the capabilities of the code to simulate a wide variety of other unsteady phenomena, e.g., the unsteady interactions between deformable or non-stationary boundaries and fluid phenomena which result in time-varying flowfields. Dynamic grids are also applicable to problems which require a grid that continuously adapts to moving discontinuities. This feature is requisite in transient problems where strong shocks can convect rapidly through the flowfield.

The dynamic grid capability has been formulated in a manner consistent with the finite-volume philosophy of the CRAFT code. We have closely followed the generalized procedure outlined by Vinokur.[32] Table IV summarizes this methodology, while additional details are given in Ref. 33. To briefly describe the procedure, the unsteady movement of the physical grid is treated purely as a geometric quantity. Therefore, unlike a finite-difference formulation where the contravariant velocity is altered such that the computational grid remains invariant in space and time, the computational grid in a finite-volume formulation varies with time. The additional flux due to the motion of the cell face is included in the flux evaulation in an upwind fashion. The conservation equations incorporate the change in the flux resulting from the time-varying cell volume as a source term. The variation of the grid with time has to be specified depending on the application. For a moving boundary, the movement of the boundary has to be related to the force balance on it. On the other hand, for a grid adapting to convecting discontinuities, the criteria for the adaption (e.g. pressure or density gradient) must be specified.

RAM ACCELERATOR STUDIES

Steady-State Simulations

It was imperative to first establish a baseline capability at the steady-state axisymmetric level to establish that CRAFT provided predictions in accord with those of other investigators.[8,11,13] With this objective in mind, predictions were generated for a projectile that was recently tested at the University of Washington's 38 mm ram accelerator test facility.

The projectile dimensions are shown in Figure 1. The tube was pressurized to 39 atm with a premixed combustible gas mixture (2.75 CH_4 + 5.8 N_2 + 2 O_2). CRAFT predictions were obtained, at the Euler non-reacting limit, for a trajectory point corresponding to a projectile flight Mach number of 3.6. A 301 x 71 curvilinear body fitted grid (shown in Figure 2) was utilized. Figures 3 and 4 show computed pressure and Mach number contours, respectively. The overall flow structure is well represented and in accord with predictions obtained by the previous investigators utilizing comparable numerics. The oblique shock structure is initiated at the projectile nose cone and causes ram compression of the reactants via a sequence of oblique shocks. The shock system weakens as it interacts with the expansion fan emanating from the projectile afterbody shoulder. Behind the projectile, a high-speed wake structure is obtained, characterized by a wake reattachment shock.

High-Pressure Compressibility Effects

Ram accelerator flowfields are characterized by extremely high pressures, caused by rapid combustion of pre-pressurized semi-stoichiometric fuel-air mixtures under near-detonative situations. Pressures in the neighborhood of 1000 atmospheres are not unusual. Under such extreme pressure conditions, high levels of compressibility are prevalent and must be accounted for during analysis.

The baseline version of CRAFT was designed for a multi-component, thermally perfect (but calorically imperfect) gaseous mixture and the perfect gas equation of state was assumed. In the RAM version, the perfect gas formulation was replaced by a virial equation of state, generalized for a multi-component mixture as summarized in Table V.

Shock tube studies indicate the importance of compressibility effects at high-pressures. Figure 5 exhibits a 10/1 shock tube solution for three different pressure ratios (10/1 atm, 100/10 atm and 1000/100 atm). Note the differences in the shock propagation pattern at the higher pressures. Shock speeds are faster at higher pressures. The steady-state case of the previous subsection was studied again with the new RAM version of CRAFT.

Table IV. Dynamic Grid Computations

EQUATIONS	$\int_{t_1} Q dv - \int_{t_1} Q dv + \int_{t_1}^{t_2} \oint_{S(t)} \vec{n} \cdot \vec{f}\, ds dt = \int_{t_1}^{t_2} \int_{V(t)} \Phi dv dt$ Term I Term II Term III Term I: PRIMARY CONSERVED VARIABLES Term II: FLUX TERMS Term III: SOURCE TERMS V(t): TIME VARYING VOLUME
METHODOLOGY	• TREAT GRID AS PURELY GEOMETRIC QUANTITY, i.e., DEFINITION OF CONTRAVARIANT VELOCITY UNCHANGED • EVALUATE FLUX TERM BY ASSUMING GRID IS HELD CONSTANT AT TIME-AVERAGED VALUE • INCLUDE ADDITIONAL FLUX ARISING FROM CELL FACE MOTION • EVALUATE SOURCE TERM FOR THE GRID AT THE NEW TIME LEVEL, THUS GIVING: $\left(\frac{Q^{n+1} - Q^n}{\Delta t}\right) V^{n+1} + Q^n \left(\frac{V^{n+1} - V^n}{\Delta t}\right) + F_n^{n+1} \bar{S} \Delta t = \Phi^{n+1} V^{n+1}$ $F_n = \vec{n} \cdot \vec{F}$, and $\bar{S}$ is the time averaged metric
NUMERICS	• SPECIFY GRID MOVEMENT AS A FUNCTION OF TIME • EVALUATE F_n AS A THIRD-ORDER UPWIND BIASED FLUX • SOLVE LINEARIZED IMPLICIT OPERATOR USING ADI PROCEDURE • USE NEWTON ITERATION FOR HIGHER ORDER ACCURACY IN TIME

Table V. Description of Gas Upgrades

THE VIRIAL EQUATION OF STATE WAS INCORPORATED FOR A MULTI-COMPONENT GAS MIXTURE

$$P = \bar{R}T \sum_n \frac{\rho_i}{w_i} \left[1 + B_m(T) \sum_n \rho_i + C_m(T) \sum_n (\rho_i)^2 \right]$$

THE SECOND AND THIRD VIRIAL COEFFICIENTS FOR THE MIXTURE ARE RELATED TO THE INDIVIDUAL SPECIES VIRIAL COEFFICIENTS.

IN GENERAL

$$B_m(T) = \sum_{ij} B_{ij} X_i X_j$$

HOWEVER, IF DATA IS UNAVAILABLE FOR CROSS COEFFICIENTS SUCH AS $B_{i\,j}$, AN APPROXIMATE RELATIONSHIP IS ASSUMED.

$$B_m(T) = \sum_i B_i Y_i$$

WHERE Y_i IS THE MASS FRACTION

Figures 6 and 7 show the computed contours of pressure and Mach number — the shocks are stronger and more closely spaced. Figures 8 and 9 compare the predictions of pressure along the tube wall and projectile afterbody from the two computations. The effect of compressibility is evident and would be more pronounced if combustion were included.

Adaptive Grid Considerations

The accurate prediction of transient ram accelerator flowfields is strongly keyed to the ability to dynamically adapt the grids to resolve the embedded shock discontinuities, wall boundary layers and separated shear layer regions. Smart logic is required to have grids evolve with the transient structure. Research has been initiated in this direction using solution adaptive gridding based on the NASA Ames SAGE adaptive solver.[34] Applications of adaptive gridding with transient/unsteady NS computations require significant experience with regard to:

a) when to implement the adaptive solver, e.g., after how many iteration steps;

b) the associated adaption parameter, e.g., a certain weighted combination of pressure, Mach number, temperature, etc.; and,

c) the control parameters, e.g., the degree of grid distortion, orthogonality, etc., per adaptive pass, etc.

The development of a suitable grid adaption strategy for ram accelerators has been initiated with focus directed towards developing rules for some of the considerations outlined above. Preliminary adaption strategies are being developed for a steady-state trajectory point analysis and will be subsequently implemented for transient calculations in a "hands-off" fashion. Figures 10 and 11 display examples of adapted grids generated for the steady-state case analyzed earlier. The grids were generated by selecting varied adaption parameters and controlling the grid distortion. Figure 12 shows the grid and resultant solution after several passes of the solution adaptive grid generator and further solution convergence with the updated grids. Compare the crispness of the shock waves with the baseline grid predictions of Figs. 3 and 4.

Finite-Rate Chemistry Considerations

Finite-rate chemistry mechanisms and rates are required for CFD simulations. Unfortunately, the vast majority of hydrocarbon kinetics data[35,36] were acquired (and mechanisms formulated) under laboratory conditions with limited (if any) applicability to the high pressure, semi-detonative ram accelerator environment. Extrapolation of kinetics data to higher pressures may lead to numerical predictions of dubious quality. Under such constraints, global multi-step mechanisms provide a useful compromise until more elaborate mechanisms can be formulated via the use of computational chemistry, as was demonstrated recently for NASP in the hypersonic scramjet environment by Cooper and coworkers at NASA Ames.

One-dimensional shock tube studies at laboratory conditions have been initiated to gain a preliminary understanding of the kinetic processes relevant to the ram accelerator. The objective of these simulations is to identify the interaction between shock formation and ignition delay in a transient environment. A related objective is to also establish an upper pressure bound for the applicability of conventional hydrocarbon kinetics rates and mechanisms. Figure 13 shows the schematic of a problem studied and the kinetic mechanism utilized for the simulations. Figures 14 and 15 show the temperature and pressure distribution in the shock tube at two instances, separated by 5μs. At the earlier time, the shock front is clearly seen (characterized by the von Neumann spike), followed by a constant pressure induction zone and subsequently the flame with rapid temperature rise. The flame front travels faster than the shock and merges with it a little later, as shown by the relatively uniform post-shock temperature. Figures 16 and 17 show the distribution of major and minor species at the two time instances considered and a consistent behavior is observed. Further one-dimensional studies with upgrades rates/mechanisms are felt to be essential for gaining an understanding of what might occur under actual ram conditions.

CONCLUDING REMARKS

This paper has described the CRAFT/RAM computer code developed for application to ram accelerator flowfields. The code developed is a specialized version of the CRAFT research code with generalized thermochemistry, advanced turbulence modeling and specialized dynamic/solution adaptive gridding capabilities. Issues pertinent to developing a fundamental understanding of the detailed physical and thermochemical processes governing ram accelerator concepts were exhibited with numerical simulations illustrating the code's capabilities to simulate these processes. Future work will include boundary layer effects (projectile and launcher tube), full transient simulations, and exploration of thermochemical issues.

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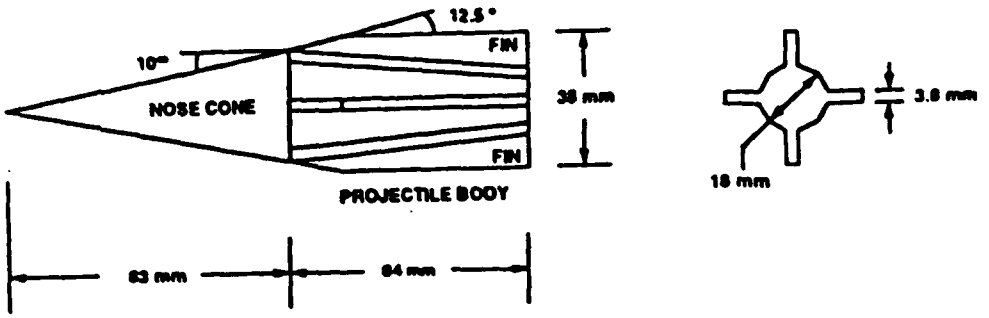


Figure 1. 38mm projectile dimensions.

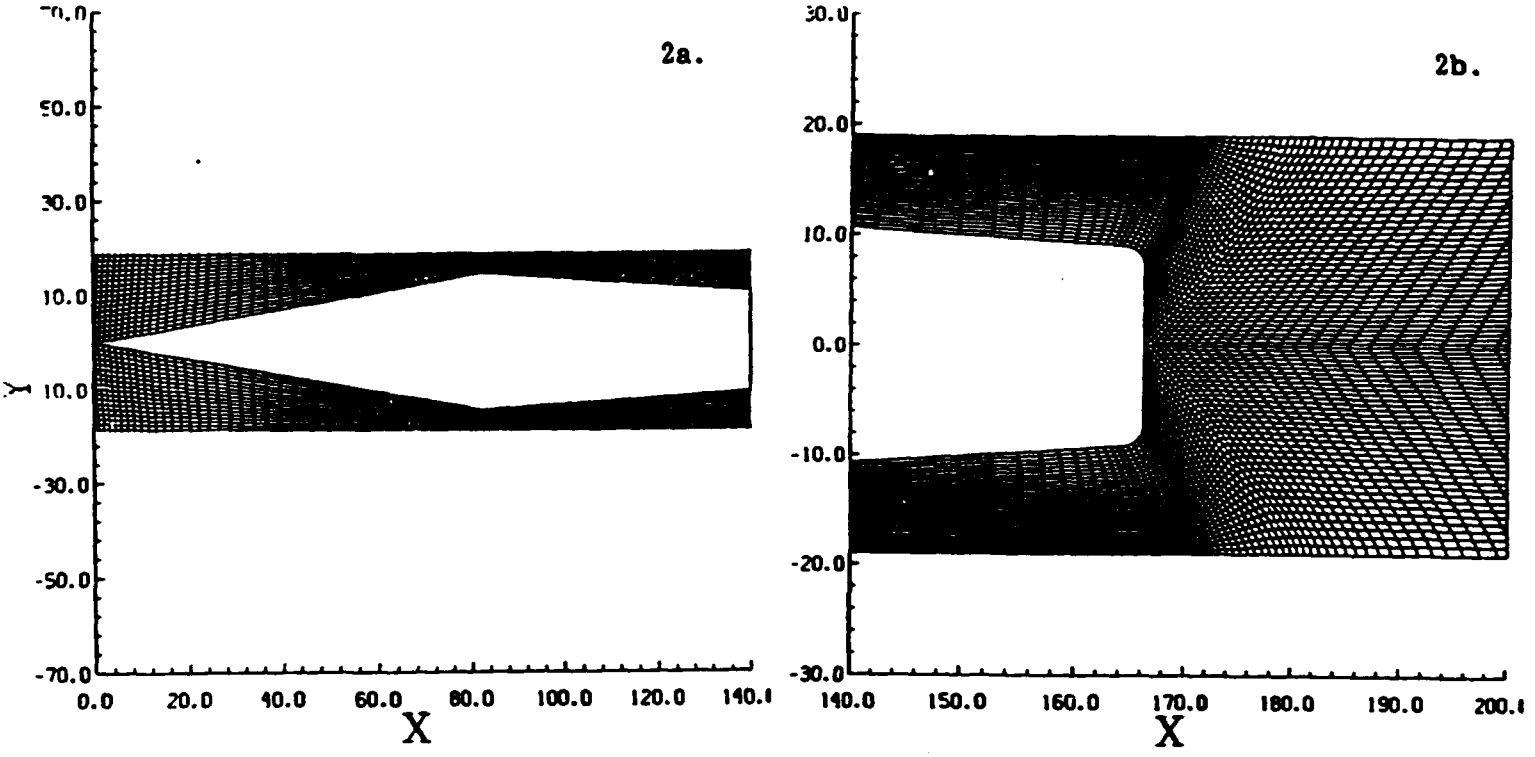


Figure 2. a) Baseline 301 x 71 curvilinear body-fitted grid, and b) Expanded view of grid in baseline region.

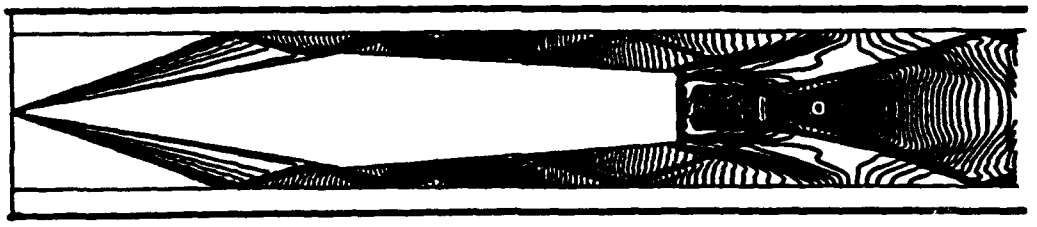


Figure 3. Computed pressure contours for 38mm projectile.

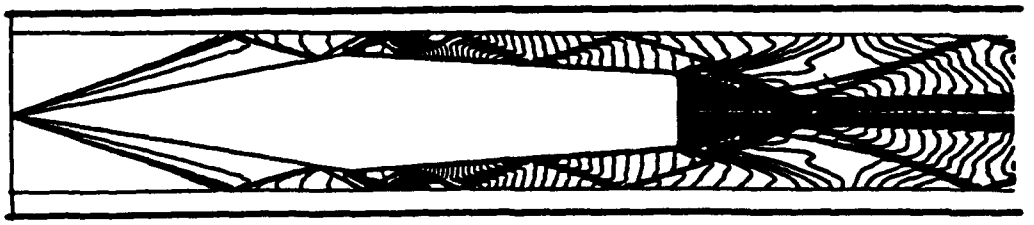


Figure 4. Computed Mach number contours for 38mm projectile.

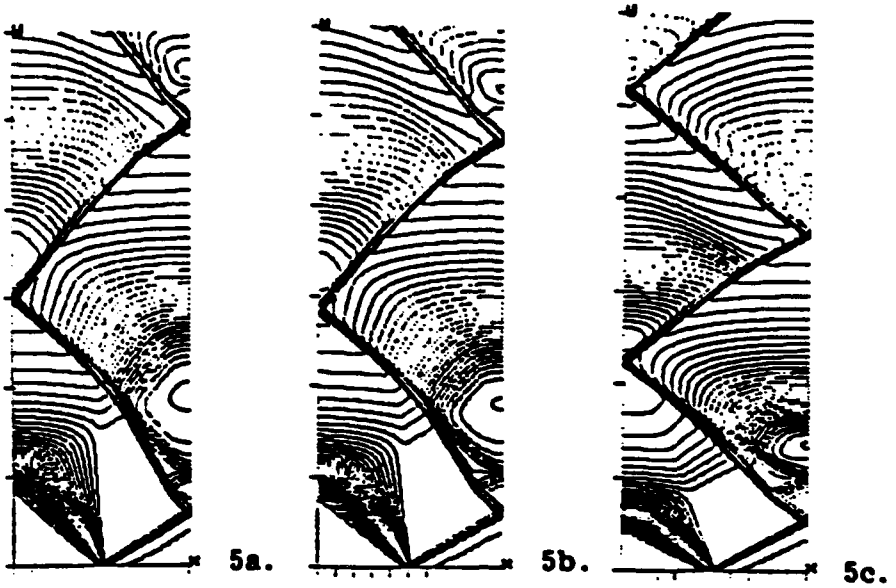


Figure 5. Pressure contours in a 10:1 shock tube at pressure ratios of: a) 10/1; b) 100/10; and c) 1000/100.

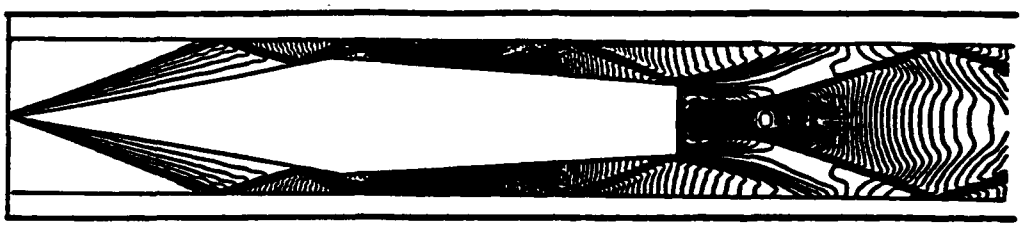


Figure 6. Computed pressure contours with Virial equation of state.

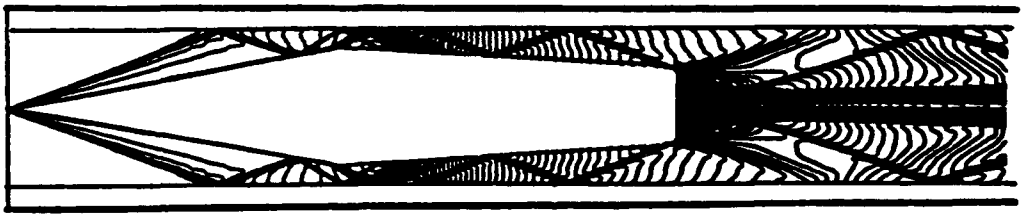


Figure 7. Computed Mach number contours with Virial equation of state.

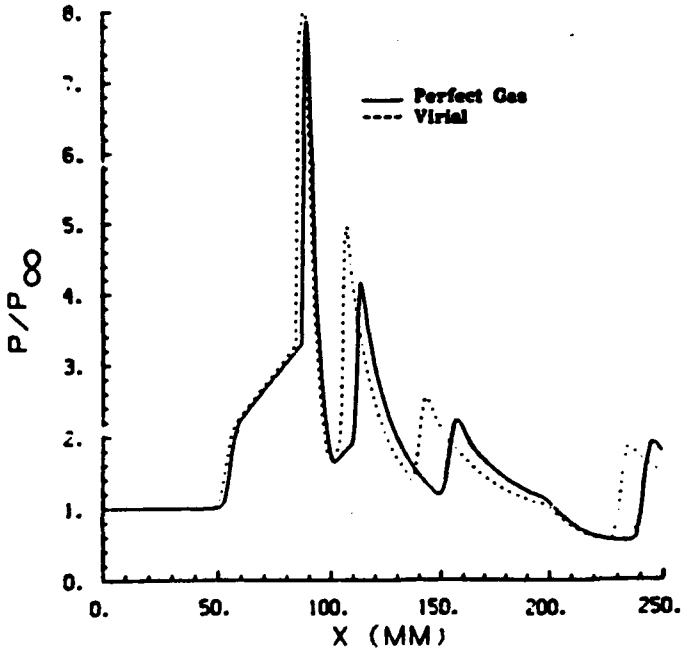


Figure 8. Comparison of tube wall pressure distribution.

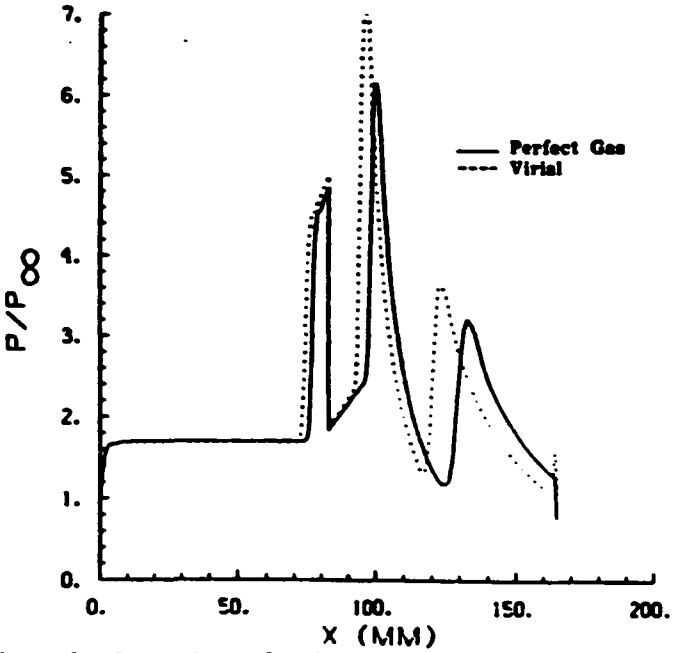


Figure 9. Comparison of projectile surface pressure distribution.

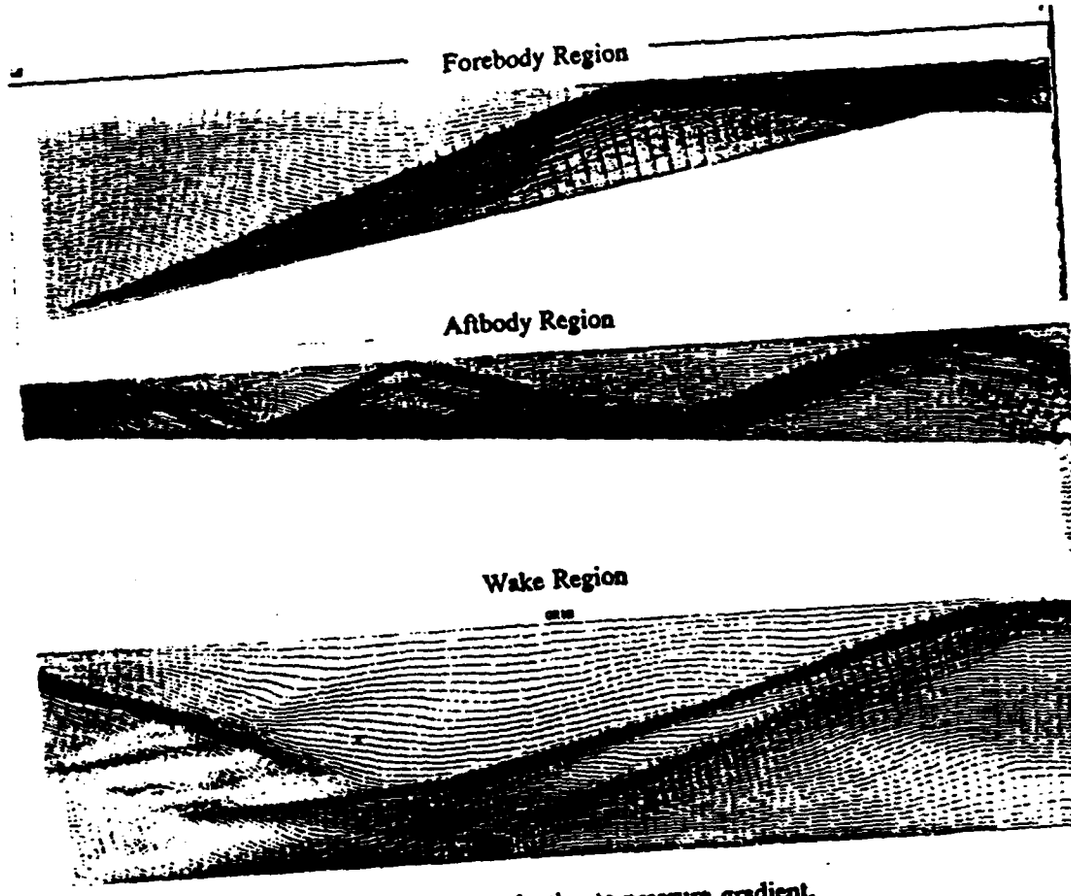


Figure 10. "Mild" adaption to pressure gradient.

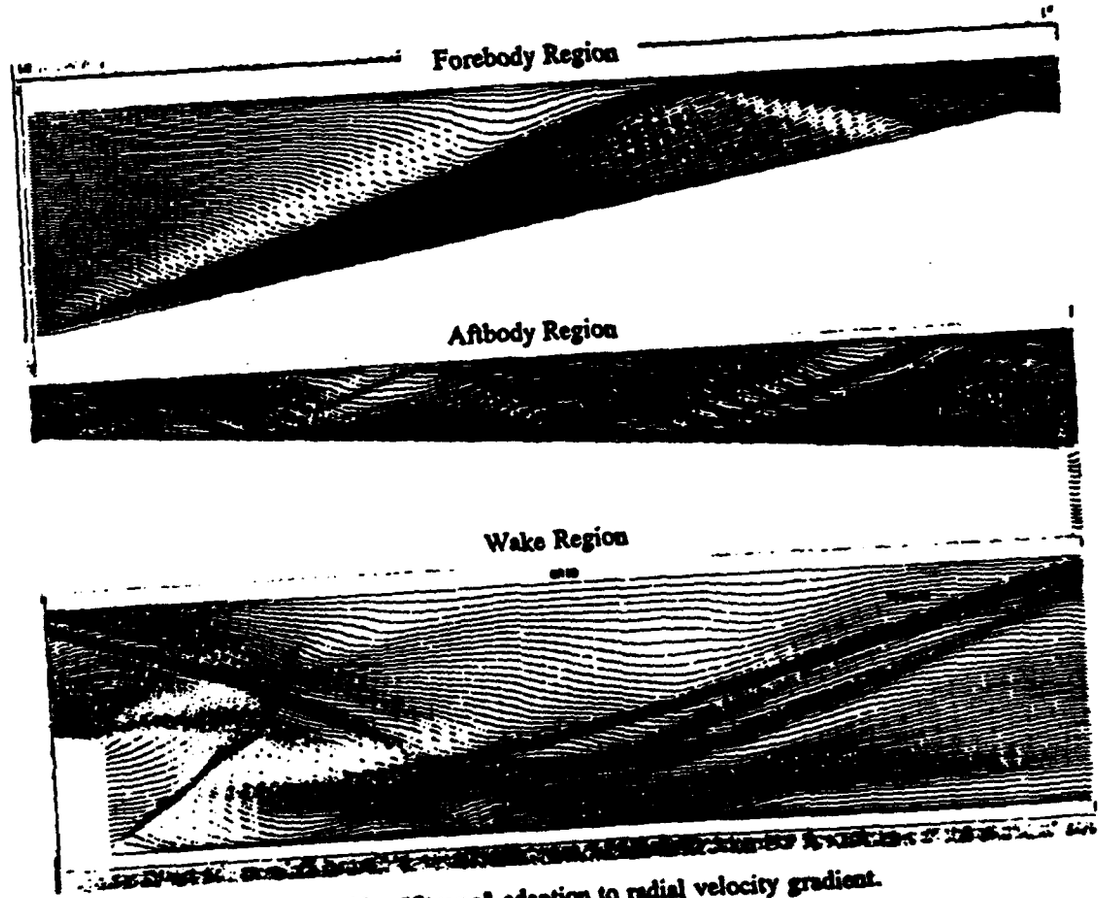
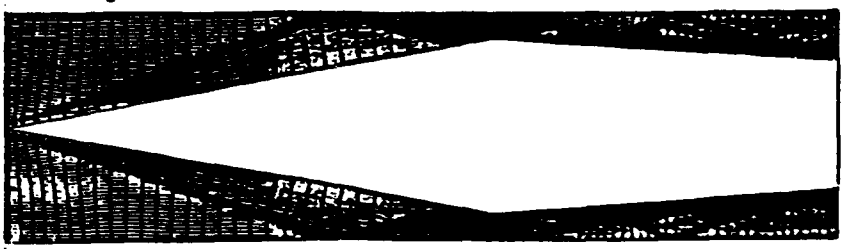
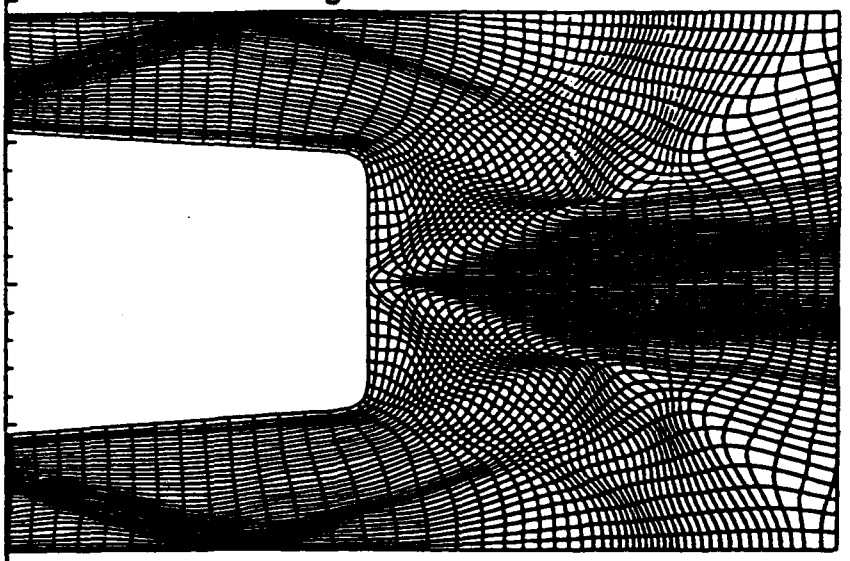


Figure 11. "Strong" adaption to radial velocity gradient.

12a.
Adapted Grid



12a.
"Zoom" of Base Region



12b. Pressure

12c. Mach Number

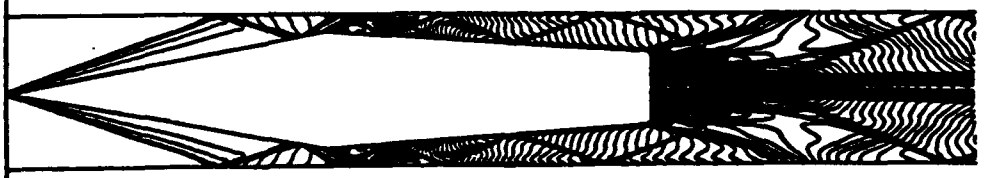
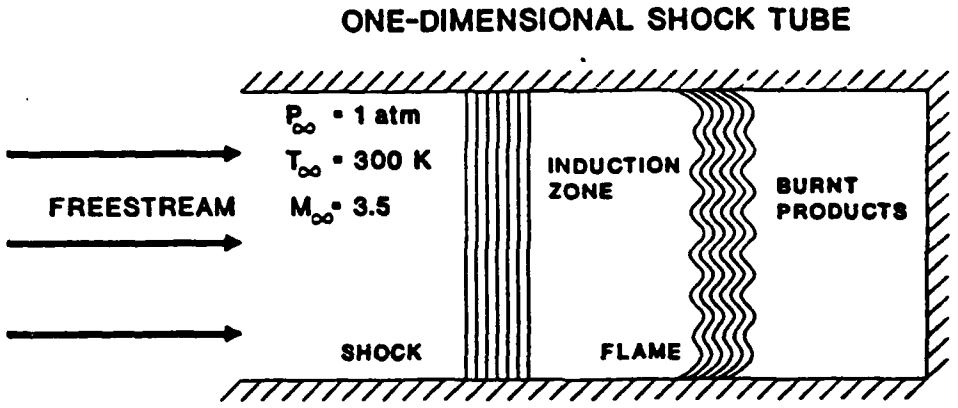


Figure 12. a) Grid obtained after multiple adaptions; b) Pressure contours on adapted grid and baseline grid; and c) Mach number contours on adapted grid and baseline grid.



METHANE REACTION MECHANISM

Reaction	k_f, rate constant
1. $CH_4 + M \rightarrow CH_3 + H + M$	$1.5 \times 10^{19} \exp(-100{,}600/RT)$
2. $CH_4 + O_2 \rightarrow CH_3 + HO_2$	$1.0 \times 10^{14} \exp(-45{,}400/RT)$
3. $O_2 + M \rightarrow 2O + M$	$3.6 \times 10^{18} T^{-1.0} \exp(-118{,}800/RT)$
4. $CH_4 + O \rightarrow CH_3 + OH$	$1.7 \times 10^{13} \exp(-8760/RT)$
5. $CH_4 + H \rightarrow CH_3 + H_2$	$6.3 \times 10^{13} \exp(-12{,}700/RT)$
6. $CH_4 + OH \rightarrow CH_3 + H_2O$	$2.8 \times 10^{13} \exp(-5000/RT)$
7. $CH_3 + O \rightarrow H_2CO + H$	$10^{13} - 10^{15}$
8. $CH_3 + O_2 \rightarrow H_2CO + OH$	$10^{11} - 10^{14}$
9. $H_2CO + OH \rightarrow HCO + H_2O$	$10^{13} - 10^{15}$
10. $HCO + OH \rightarrow CO + H_2O$	$10^{12} - 10^{15}$
11. $CO + OH \rightarrow CO_2 + H$	$3.1 \times 10^{11} \exp(-600/RT)$
12. $H + O_2 \rightarrow OH + O$	$2.2 \times 10^{14} \exp(-16{,}600/RT)$
13. $O + H_2 \rightarrow OH + H$	$4.0 \times 10^{14} \exp(-9460/RT)$
14. $O + H_2O \rightarrow 2OH$	$8.4 \times 10^{14} \exp(-18{,}240/RT)$
15. $H + H_2O \rightarrow H_2 + OH$	$1.0 \times 10^{14} \exp(-20{,}400/RT)$
16. $H + OH + M \rightarrow H_2O + M$	$2.0 \times 10^{1} T^{-1.0}$
17. $CH_3 + O_2 \rightarrow HCO + H_2O$	$10^{11} - 10^{12}$
18. $HCO + M \rightarrow H + CO + M$	$2.0 \times 10^{13} T^{1/2} \exp(-28{,}800/RT)$

Figure 13. Reactive shock tube schematic and methane kinetic mechanism.

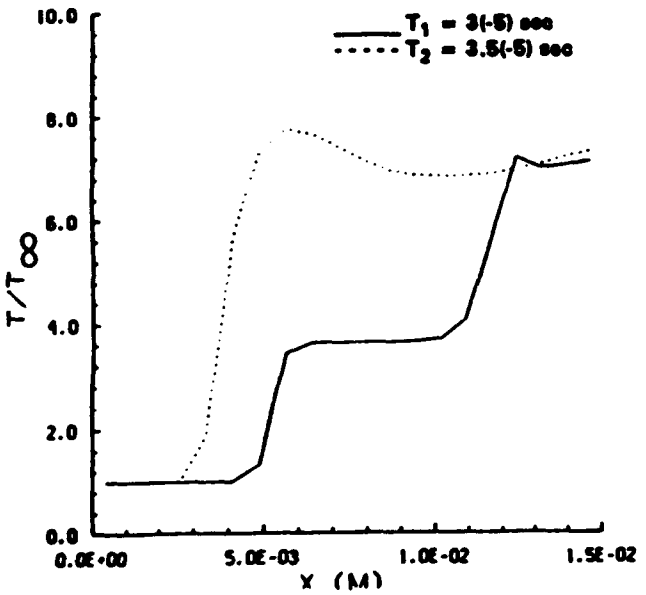


Figure 14. Temperature distribution in shock tube at two time instances.

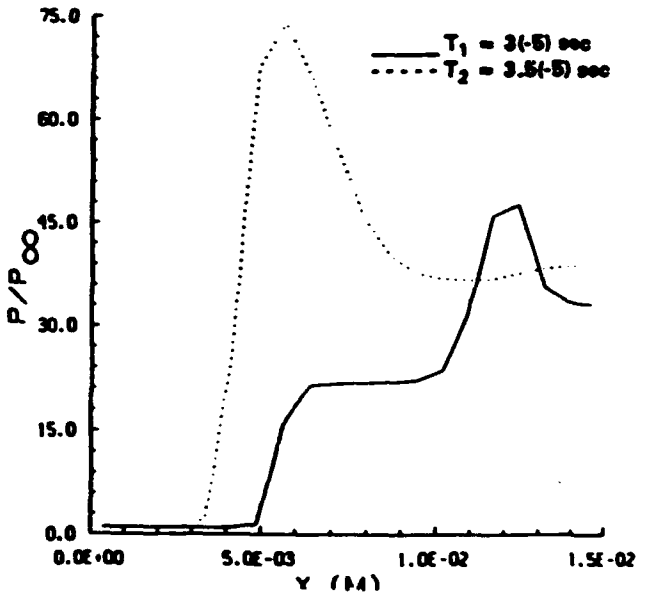


Figure 15. Pressure distribution in shock tube at two time instances.

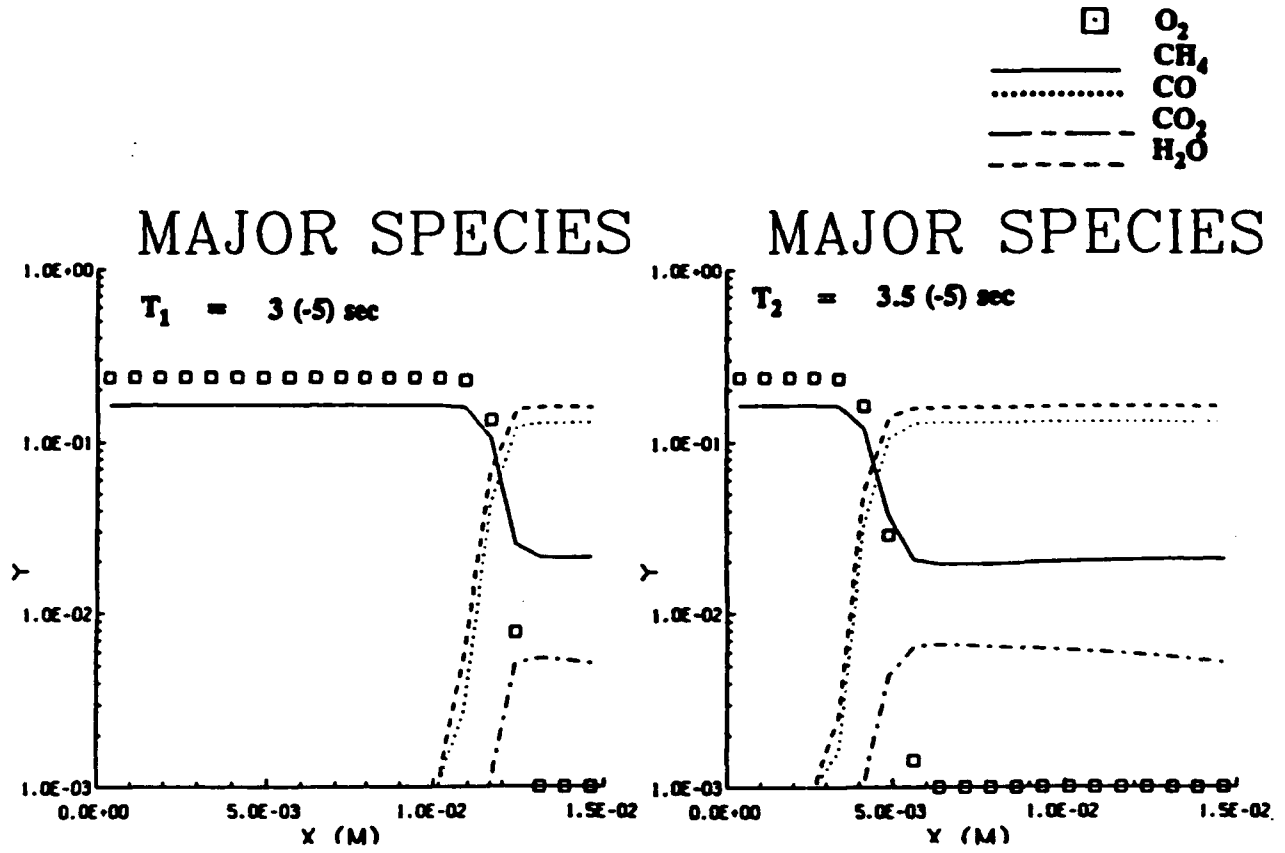


Figure 16. Major species distribution in shock tube at two time instances.

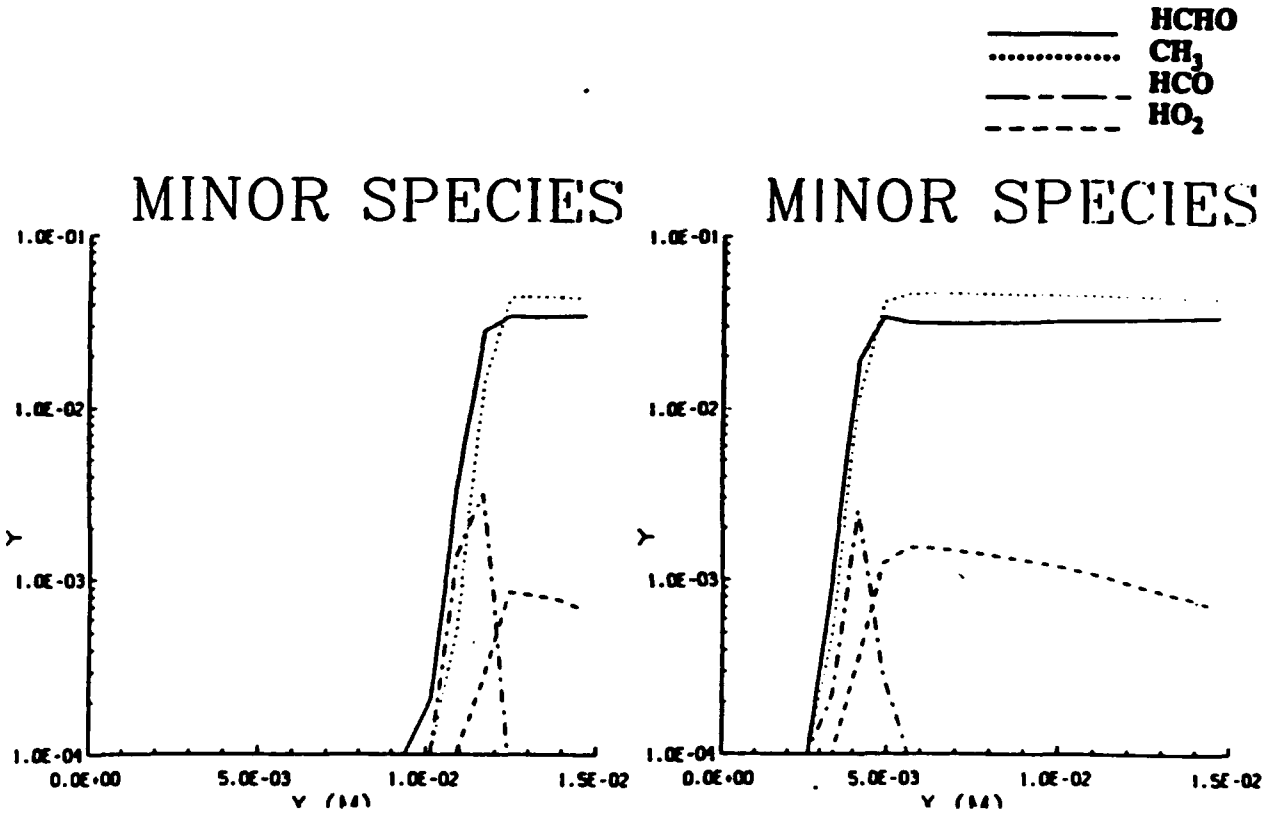


Figure 17. Minor species distribution in shock tube at two time instances.

Distribution
WL-TP-92-015

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Attn: DTIC-DDAC
Cameron Station
Alexandria VA 22304-6145
2

AUL/LSE
Maxwell AFB AL 36112-5564
1

AFSAA/SAI
Washington DC 20330-5420
1

WL/FIES/SURVIAC
Wright-Patterson AFB OH 45433-6553
1

Eglin AFB offices:
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WL/MNOI (Scientific and Tech. Info. Facility) 1
WL/MNGS 4

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